AFRL-ML-WP-TP-2006-483

MESOSCALE MODELING OF THE RECRYSTALLIZATION OF WASPALOY AND APPLICATION TO THE SIMULATION OF THE INGOT-COGGING PROCESS (PREPRINT)

Jean-Philippe Thomas
S.L. Semiatin

SEPTEMBER 2006

Approved for public release; distribution is unlimited.

STINFO COPY

MATERIALS AND MANUFACTURING DIRECTORATE
AIR FORCE RESEARCH LABORATORY
AIR FORCE MATERIEL COMMAND
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7750

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
September 2006	Conference Paper Preprint	N/A

4. TITLE AND SUBTITLE
MESOSCALE MODELING OF THE RECRYSTALLIZATION OF WASPALOY AND APPLICATION TO THE SIMULATION OF THE INGOT-COGGING PROCESS (PREPRINT)

5a. CONTRACT NUMBER
In-house

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
62102F

6. AUTHOR(S)
Jean-Philippe Thomas (UTC)
S.L. Semiatin (AFRL/MLLMP)

5d. PROJECT NUMBER
4349

5e. TASK NUMBER
L0

5f. WORK UNIT NUMBER
VT

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Universal Technology Corporation
1270 North Fairfield Road
Dayton, OH 45432

Processing Section, Metals Branch (AFRL/MLLMP)
Metals, Ceramics, and Nondestructive Evaluation Division
Materials and Manufacturing Directorate
Air Force Research Laboratory, Air Force Materiel Command
Wright-Patterson Air Force Base, OH 45433-7750

8. PERFORMING ORGANIZATION REPORT NUMBER
AFRL-ML-WP-TP-2006-483

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Materials and Manufacturing Directorate
Air Force Research Laboratory
Air Force Materiel Command
Wright-Patterson AFB, OH 45433-7750

10. SPONSORING/MONITORING AGENCY ACRONYM(S)
AFRL-ML-WP

11. SPONSORING/MONITORING AGENCY REPORT NUMBER(S)
AFRL-ML-WP-TP-2006-483

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES
The U.S. Government is joint author of this work and has the right to use, modify, reproduce, release, perform, display, or disclose the work.

Conference paper submitted to the Proceedings of the Materials Science and Technology 2006 Conference and Exhibition, MS&T organizers. PAO Case Number: AFRL/WS 06-1440, 07 Jun 2006.

14. ABSTRACT
Typical models of recrystallization based on the Avrami formulation cannot be applied to cases characterized by anisotropic material behavior (e.g., hot working of ingot structures) or several consecutive waves of partial dynamic and/or metadynamic recrystallization (as in multi-hit deformation). The primary processing of ingots by cogging poses challenges with regard to both of these aspects. The present work reports on a new meso-scale, mechanism-based model that has been developed for such problems and applied initially for Waspaloy. The model formulation comprises two main parts: a geometric framework and a set of equations that describe microstructure evolution due to the various driving forces. The geometric framework is based on so-called meso-structure units (MSUs), each of which represents an aggregate of similar grains. The MSUs evolve via nucleation-and-growth processes quantified by equations describing energy storage, nucleation, and grain-boundary migration. The model was tested on a prototypical cogging process using 3D-FEM simulations.

15. SUBJECT TERMS
recrystallization, superalloys, Waspaloy, cogging, modeling

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT:	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON (Monitor)
a. REPORT	b. ABSTRACT	c. THIS PAGE			S.L. Semiatin
Unclassified	Unclassified	Unclassified	SAR	18	19b. TELEPHONE NUMBER *(Include Area Code)* N/A

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39-18

Mesoscale Modeling of the Recrystallization of Waspaloy and Application to the Simulation of the Ingot-Cogging Process

Jean-Philippe Thomas* and S. L. Semiatin

Air Force Research Laboratory, Materials and Manufacturing Directorate,
AFRL/MLLM, 2230 Tenth Street, Wright-Patterson Air Force Base, OH 45433
*Universal Technology Corporation, 1270 North Fairfield Road, Dayton, OH 45432

Keywords: Recrystallization, superalloys, Waspaloy, cogging, modeling

Abstract

Typical models of recrystallization based on the Avrami formulation cannot be applied to cases characterized by anisotropic material behavior (e.g., hot working of ingot structures) or several consecutive waves of partial dynamic and/or metadynamic recrystallization (as in multi-hit deformation). The primary processing of ingots by cogging poses challenges with regard to both of these aspects. The present work reports on a new meso-scale, mechanism-based model that has been developed for such problems and applied initially for Waspaloy. The model formulation comprises two main parts: a geometric framework and a set of equations that describe microstructure evolution due to the various driving forces. The geometric framework is based on so-called meso-structure units (MSUs), each of which represents an aggregate of similar grains. The MSUs evolve via nucleation-and-growth processes quantified by equations describing energy storage, nucleation, and grain-boundary migration. The model was tested on a prototypical cogging process using 3D-FEM simulations.

Introduction

High-strength, high-temperature superalloys, such as Waspaloy, 718, and, more recently, 720 and 718Plus™, have a variety of uses in aircraft engines. Thus, the thermomechanical processing (TMP) of these materials has been the subject of extensive investigation aimed at enhancing their properties as well as reducing manufacturing cost. For the vast majority of components made from these alloys, typical manufacturing processes still involve a complex sequence of melting/remelting, homogenization, and numerous hot working steps. The modeling of microstructure evolution at every stage from the primary processing of an ingot to the final close-die forging of a specific component represents an important challenge to the aerospace industry. Two main approaches have been used to meet this need - phenomenological and mechanism-based models.

Phenomenological microstructure-evolution models, such as those based on the Avrami formulation, have achieved great success over the past decades. However, they fail to address some important issues. First, these models can usually be applied only to specific, relatively-narrow ranges in terms of initial microstructure, temperature, strain, and strain rate which have been characterized experimentally. As a consequence, microstructure prediction for an entire process may involve a succession of different models, invariably leading to the loss of accuracy from one process step to the next. In addition, a new model and associated experiments are required each time a new processing route is investigated. Second, the use of phenomenological formulations becomes questionable as process complexity increases. For a

single deformation followed by a reheat, for example, fitting of measurements using an Avrami approach often gives reasonable results even if the nucleation-and-growth assumptions underlying such formulations are not satisfied. By contrast, the shortcomings of phenomenological models become most noticeable for multi-step processes involving consecutive waves of partial dynamic and/or metadynamic recrystallization, when precipitation occurs, or anisotropy effects become important. All of these features pertain to ingot cogging because of the multi-hit, multi-reheat nature of the process, which gives rise to multiple generations of grains of various sizes and levels of work-hardening. Furthermore, the temperature at the periphery of the ingot can drop below the solvus due to die chill, and the initial microstructure usually exhibits highly-anisotropic properties due to both microstructural (i.e., columnar grains) and crystallographic (strong <100> solidification) texture. One final challenge in the use of phenomenological methods pertains to the difficulty in correlating data for different alloys in a given class (such as gamma-gamma prime superalloys), let alone results for the same material, obtained by different investigators due to the lack of a firm physical basis in the modeling approach.

Physics-based models, such as cellular-automata and Monte-Carlo techniques, have been under development for a number of years to provide a better description of microstructure evolution during thermomechanical processing. Despite their strengths, these models would require excessive computation power if applied at every node in a finite-element-method (FEM) simulation of a hot-working problem such as ingot cogging. As such, conventional physics-based models can be applied to gain insight into behavior only at selected local regions, or tracking points, in an FEM simulation.

The present paper summarizes research whose objective was to develop a modeling approach which combines the relative simplicity of phenomenological approaches, thus enabling application in FEM codes, but nonetheless includes important aspects of the physics of microstructure evolution. The specific approach focused on the formulation of a novel meso-scale, mechanism-based model of dynamic and metadynamic recrystallization and its application to the TMP of superalloys such as Waspaloy. This new approach comprised two main parts: a geometric framework and a set of equations that describe the (main) driving forces of microstructure evolution. This work is summarized first. Subsequently, the validation of the coupled meso-scale + FEM model using a prototypical ingot-cogging process is briefly described.

I. Geometric Framework of the Meso-Scale Model

Among the variables that comprise the mathematical representation of a microstructure, a subset constitutes its geometric description. These geometric variables, such as grain size, change during microstructure evolution. In particular, volume conservation is a central issue during the modeling of recrystallization because the growth of a grain has to be compensated by the equal volume loss of another. In the Avrami formulation, this problem is relatively simple inasmuch as when some areas of recrystallized grains impinge, their boundaries stop migrating. Such an assumption fits the behavior expected for static recrystallization, but becomes questionable during metadynamic recrystallization, not to mention dynamic recrystallization. Nevertheless, this shows that in addition to a geometric description which is somewhat of a “static” concept, a model of microstructure evolution requires a geometric framework in which both the geometric variables (grain sizes, volume grain densities, etc.) and the geometric laws of grain interaction are included. The present framework was designed such that it responds to two kinds of input: nucleation rates and grain-boundary velocities which are described by driving forces equations in association with the remaining variables of microstructure description.

Description of the Geometric Framework

Because the model is to be applied at each node of a 3D-FEM simulation, it should require modest computational power. Therefore, instead of representing every grain, the microstructure description relies on averaging over grain populations that are characterized by similar properties and are expected to exhibit similar evolution. This requirement leads to the definition of grain families referred to as meso-structure units, or MSUs, on which the geometric framework is based. To deal with recrystallization, at least two MSUs are necessary: one for the initial grains and another for the recrystallized ones. In the case of multi-hit deformation, such as during cogging, at least two generations of recrystallized grains are required: one for the grains that appeared during previous hits, which may have grown and then stored some energy again, and those that nucleated during the current or latest deformation. For the work described later (for Waspaloy), five MSUs are allocated. The first two (indices 0 and 1) represent initial grains of average/high Taylor factor (M_T) and those that have a very low M_T. MSUs denoted with indices 2 and 3 are for previously recrystallized grains with the same distinction based on the Taylor factor. The last MSU (index 4) comprises the grains that appeared during the current deformation from nuclei generated by the four other MSUs and those it generates itself.

The first input of the geometric framework includes the nucleation rates of each MSU and the size of the nuclei; the latter is supposed to be the same in every MSU. The volume of each nucleus is subtracted from that of the MSU in which it appeared and added to the volume of the fifth MSU to insure volume conservation. Grain-boundary surfaces of nuclei are transferred also. The simultaneous increase of volume and corresponding grain-boundary surface of all the nuclei lead to an increase in the grain density of the last MSU and to a reduction of its grain size. The description of the operations related to nucleation by this geometric framework is relatively straightforward.

After recrystallized grains have appeared, they grow because their stored energy is lower than that of the grains of the four other MSUs which are consumed. This growth is described by the second input of the geometric framework, which consists of the migration rate of the boundaries separating each pair of MSUs. To translate these migration velocities into rates of volume change, the statistical probability for surface contact between grains of different MSUs must be determined. For the simple case of isotropic grains (spheres) of size D_i and volume density n_i for MSU *i*, the surface area of grain *i* and the fraction of the boundary of a grain that is in contact with grains of MSU *j* is given as follows:.

$$s_i = \pi D_i^2 \tag{1}$$

$$q_j = \frac{n_j s_j}{\sum_{k=0}^{N_{MSU}-1} n_k s_k} = \frac{n_j s_j}{S_{total}} \tag{2}$$

The rate of change of the volume of the grains of MSU *i* due to their interaction with grains of MSU *j*, where $\dot{u}_{ij}$ denotes the velocity of a grain *i* – grain *j* boundary, is

$$\dot{v}_{ij} = q_j s_i \dot{u}_{ij} = \frac{n_j s_j}{S_{total}} s_i \dot{u}_{ij} \tag{3}$$

Other, somewhat more complex, expressions have been developed for the case of anisotropic (ellipsoidal) grains and further enhanced to deal with the development of *intragranular* recrystallized areas due to particle-simulated nucleation such as occurs during the recrystallization of Waspaloy ingots [1, 2].

Test Examples for the Geometric Framework

The geometric framework was tested with simple inputs in order to evaluate its behavior prior to applying it to problems with complex, physically-realistic, driving forces. First, a few values of nucleation rates and boundary velocities were chosen such that the strain for 50 pct. recrystallization was obtained in each case at a deformation of ~0.5 for an initial grain size of 100μm (Figure 1a). Such balance between nucleation and boundary migration sheds light on the effect of strain rate on dynamic-recrystallization (DRX) behavior. The Avrami exponents lay between 1 and 3. The second set of test cases dealt with an ingot microstructure in which the volume density of particles at which particle-simulated nucleation (PSN) can occur was varied for a fixed nucleation rate and grain-boundary velocity (Figure 1b). An increase in the density of PSN sites led to an increase in the overall recrystallization kinetics as well as the Avrami coefficient, as has been observed experimentally [1].

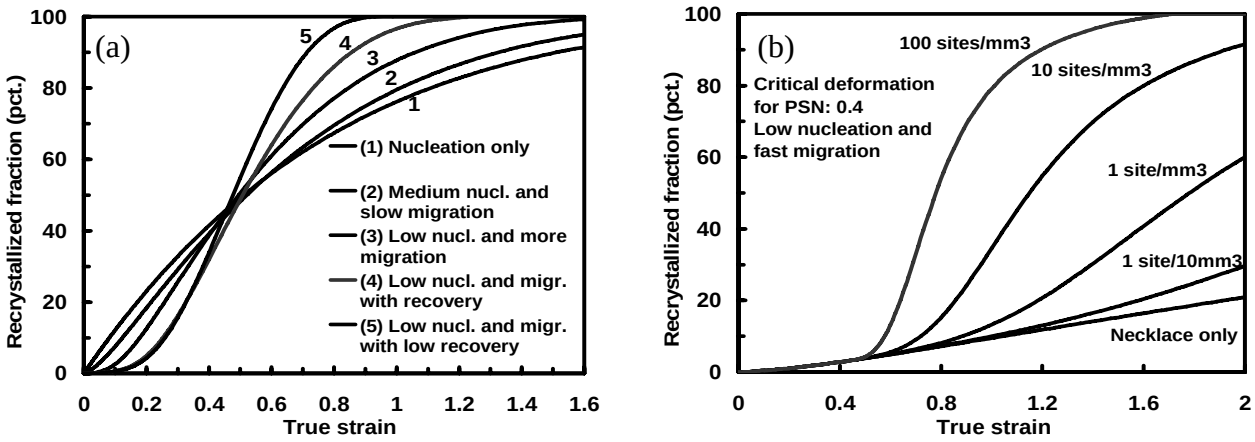

Figure 1. Response of the geometric framework to simple inputs for (a) wrought microstructures deformed with various nucleation rates (1 nucleus per 2.5, 10, 100 μm^2 of grain boundary and per unit strain) and boundary-migration rates (0, 25, 45, up to 80, up to 180 μm per unit strain), (b) ingot microstructures with various densities of PSN sites with a nucleation rate of 1 nucleus per 100 μm^2 of grain boundary and per unit strain and a boundary velocity of 100 μm per unit strain.

II. Driving Forces and Solution Method

In addition to the geometric variables, a few variables used for the evaluation of the driving forces for recovery, recrystallization, and grain growth are associated with each MSU. These variables are primarily the dislocation density (ρ_i), two sub-boundary densities (one for sub-boundaries located near the grain periphery (S_{sbi}) and the other for those dispersed within the volume (S_{sbvi})), two parameters that quantify the overall disorientation of each sub-boundary population (denoted x_i and x_{vi}, respectively), and the Taylor factor M_{Ti}. The driving-force expressions and the determination of the order of magnitude of some of the physical parameters for Waspaloy are summarized below.

Static Grain Growth

Even though it usually follows recovery and recrystallization (i.e., after dislocation-related driving forces are eliminated), static grain growth is also the simplest process and hence is summarized first here. The driving force P is simply related to boundary energy γ and grain diameter D, i.e.,

$$P = \frac{\gamma}{2D} \tag{4}$$

The grain-boundary mobility is assumed to be expressed as follows:

$$M = M_0\left(\frac{P}{P_0}\right)^{\lambda} \tag{5}$$

in which λ is a material constant, and P_0 is a reference driving force (for the static grain growth of a 1-μm grain size). When the driving force is equal to P_0, the grain boundary mobility is M_0. The general law of static grain growth is then

$$D^{\lambda+2} - D_0^{\lambda+2} = kt \tag{6}$$

in which t denotes time, k is a coefficient that depends on temperature, and D_0 is the initial grain size.

Experimental data suggest that the actual relation for the static grain growth of Waspaloy (with grain size expressed in microns) is as follows [3]:

$$D^3 - D_0^3 = 2*10^{26}\exp\left(-\frac{595000}{RT}\right)t \tag{7}$$

A comparison of Equations (6) and (7) indicates that λ=1, which quantifies the effect of solutes on boundary migration. A comparison of Equations (5), (6), and (7) leads to the following expression for M_0 (in $m^4/J/s$):

$$M_0 = 6.35*10^{13}\exp\left(-\frac{595000}{RT}\right) \tag{8}$$

Dislocation Density Evolution during Metadynamic Recrystallization

The determination of the velocity of the boundary between initial and recrystallized grains during *metadynamic* recrystallization was used to estimate of the dislocation density that is necessary to provide the driving force required to obtain such a velocity in conjunction with the grain-boundary mobility determined above. To this end, a model based on the Avrami formulation was solved with the constraint of continuity from the dynamic to the metadynamic regime, viz.,

$$X_{dyn} = 1 - \exp\left(-\ln(2)\left(\frac{\varepsilon - 0.17}{\varepsilon_{0.5}}\right)^{4.2}\right) \tag{9}$$

$$X_{m-dyn} = X_{dyn} + \left(1 - X_{dyn}\right)\left[1 - \exp\left(-\ln(2)\left(\frac{t}{t_{0.5}}\right)\right)\right] \tag{10}$$

The strain and time for 50 pct. dynamic recrystallization of Waspaloy are given by the following relations:

$$\varepsilon_{0.5} = 4.6*10^{-5}\exp\left(\frac{110000}{RT}\right)\dot{\varepsilon}^{0.078} \tag{11}$$

$$t_{0.5} = 8*10^{-7}\exp\left(\frac{160000}{RT}\right)\varepsilon^{0.388}\,\dot{\varepsilon}^{0.06}\,D_0^{0.387} \tag{12}$$

Because the recrystallized fraction and the average size of the remnants of the initial grains are interrelated, the time derivative of the metadynamic-recrystallized fraction provides an estimate of the velocity of interfaces between the initial and recrystallized grains:

$$\dot{u} = \frac{2D_0}{3} \frac{\dot{X}_{m-dyn}}{\left(1 - X_{m-dyn}\right)^{2/3}} \tag{13}$$

The relation for the jump in stored energy across a growing recrystallization nucleus ($P \sim \rho G b^2/2$) combined with the expression for the grain-boundary mobility (Equation (5) with $\lambda=1$) gives the following equation for the dislocation density during metadynamic recrystallization:

$$\rho = \frac{2}{Gb^2} \sqrt{\frac{\dot{u}\, P_0}{M_0}} \tag{14}$$

Using the data collected by Shen [3] for metadynamic recrystallization of wrought Waspaloy, a marked dependence of dislocation density on time (t) and temperature was found (Figure 2). An extrapolation of the trend lines back to t = 0 gives dislocation densities of approximately 5 x 10^{13}m^{-2} and 2 x 10^{13}m^{-2} at the end of deformation at 1066°C and 1121°C, respectively.

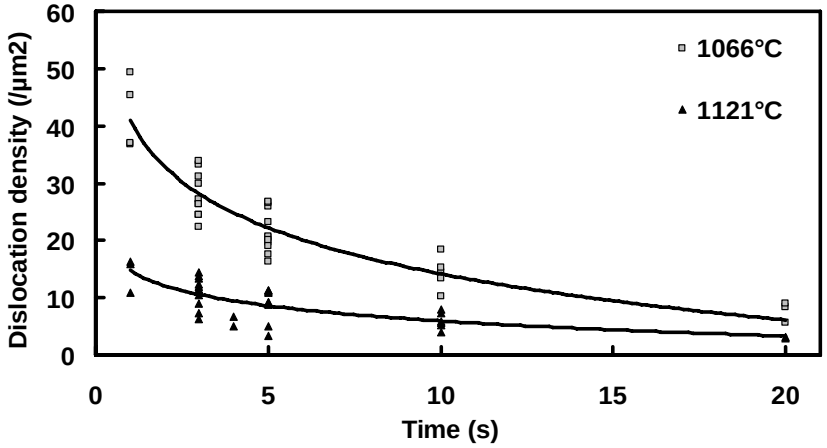

Figure 2. Evolution of dislocation density during metadynamic recrystallization for wrought Waspaloy.

Dislocation Density Evolution during Deformation

Various expressions have been proposed for strain hardening and dynamic recovery in literature. The most commonly used is the Laasraoui-Jonas expression [4], which assumes a constant mean free path of dislocations and a dynamic recovery rate linearly proportional to the instantaneous dislocation density. However, these expressions tend to give flow curves with a rounded shape during the early stage of deformation. Such a behavior has been observed for some steels deformed in the austenite field, but it is not representative of observations for Waspaloy, which exhibits a rather steep and linear initial stress-strain response (Fgure 3a). In contrast to the Laasraoui-Jonas model, flow curves which have a linear initial portion are obtained from the Kocks-Mecking formulation, which is based on the assumption that the mean free path of dislocations is proportional to the average distance between forest dislocations, and which was successfully applied elsewhere in the case of superalloy 718 [5].

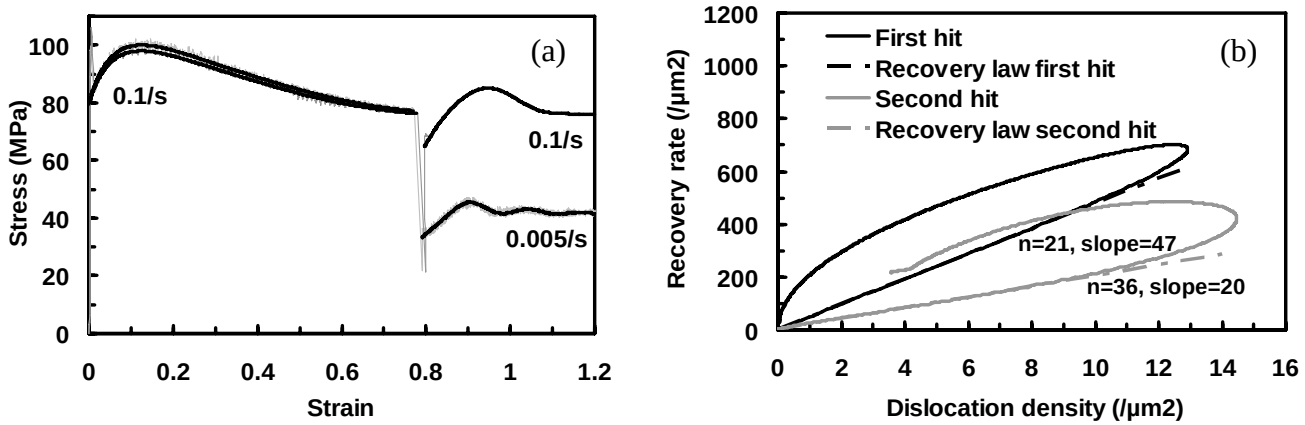

Figure 3. (a) Stress-strain curves and (b) apparent recovery rates for wrought Waspaloy deformed in uniaxial compression at 1177°C in two hits separated by a 3-second hold time.

In such a case, one can define the average number n of forest dislocations crossed before a mobile dislocation stops contributing to deformation; the rate of dislocation generation is then given by

$$\dot{\rho}^{+} = \dot{\varepsilon}\frac{\sqrt{\rho}}{nb} \tag{15}$$

If the classic expression for stress is applied, i.e.,

$$\sigma = \sigma_0 + \alpha G b\sqrt{\rho} \tag{16}$$

it can be shown that the apparent recovery rate of the microstructure can be estimated as follows

$$\frac{d\rho^{-}}{d\varepsilon} = \frac{\sigma - \sigma_0}{\alpha G b^2}\left(\frac{1}{n} - \frac{2}{\alpha G}\frac{d\sigma}{d\varepsilon}\right) \tag{17}$$

The application of Equation (17) to the Waspaloy flow curves (Figure 3a) reveals a long linear dependence of the apparent recovery rate on the dislocation density (Figure 3b), suggesting that the dynamic recovery rate is indeed proportional to dislocation density, as in the Laasraoui-Jonas formulation. This behavior can be interpreted as the annihilation of dislocation dipoles. The increase of the apparent recovery rate above the linear initial regime is the signature of dynamic recrystallization, which is known to be responsible for an additional softening term.

Figure 3b also shows that the maximum dislocation density developed *during* hot working of Waspaloy at 1177°C is ~1.5 x 10^{13}m^{-2}, which is consistent with the order of magnitude deduced above from the analysis of the growth of pre-existing nuclei during metadynamic recrystallization at 1066°C and 1121°C, i.e., 5 x 10^{13}m^{-2} and 2 x 10^{13}m^{-2}, respectively. The ability of such a physically-based model to unify behaviors from the dynamic regime to static grain growth, including metadynamic evolution, is thus a great improvement compared to phenomenological approaches and offers the promise of a significantly more robust description of microstructure evolution both within the domain of the measurements from which its parameters were determined as well as perhaps slightly beyond this regime.

Sub-boundary Generation/Disorientation and Nucleation

Nucleation is a very complex process that can involve numerous mechanisms. To mention just a few, these mechanisms include the bulging of initial boundaries [6, 7], twin boundary generation/disorientation [7], the development of a critical nucleus radius depending on the surrounding

stored energy [8], thermodynamic analysis and entropy aspects [9], treatments dealing with the correlation between the crystallographic orientations of the nucleus and parent grain [6], etc. Depending on the specific alloy, the experimental tools used, or the thermomechanical route by which nuclei are generated, the combination of the various mechanisms can result in very different nucleation behaviors, observations, and modeling considerations.

In the present work, the nucleation process was modeled based on what appears to be the controlling mechanism for superalloys. Previous observations for superalloy 718 [10] and the occurrence of PSN [1] led to the conclusion that the primary nucleation mechanism for recrystallization in Waspaloy is associated with the development of strain incompatibilities. Such incompatibilities are responsible for the generation and disorientation of sub-boundaries, which eventually leads to local crystallographic rotation of some sub-grains that become nuclei. Such areas are located near initial grain boundaries, where incompatibilities of deformation between neighboring grains are accommodated, as well as around particles that disturb the deformation field. This physical picture of nucleation implicity incorporates other related mechanisms. For instance, when the crystallographic rotation of a sub-grain leads to the formation of a new nucleus, nucleation could be interpreted in terms of a critical radius/energy criterion. However, because crystallographic rotation occurred, high local energy around the nucleus can be expected to prevent it from collapsing and make it grow.

Given the complexity of the processes that describe the development of strain incompatibility and dynamic recovery which control sub-boundary generation and disorientation (eventually leading to formation of mobile high angle grain boundaries that form the actual nuclei), the specific relations that were chosen to describe substructure evolution and nucleation are quite empirical based and still in need of substantial improvements. In particular, in the present work, two populations of sub-boundaries are represented depending on their location within the grains and, as a consequence, on the location of the nucleation sites they provide. The first population is responsible for nucleation near the initial grain boundaries, whereas the second is the source of PSN. For each of these populations, three driving force equations are used. The first equation is for sub-boundary generation, the second gives the sub-boundary disorientation, and the last aims at representing the kinetics of sub-boundary conversion into mobile, high-angle boundaries. The result of the latter equation is converted into a nucleation rate through the use of critical nucleus size or, more exactly, nucleus surface. As an illustration, the equations used for volume sub-boundaries are the following:

$$\dot{S}_{sbV}^{+} = k_{GV} \exp\left(\frac{Q_{GV}}{RT}\right) \dot{\varepsilon} F_V \left(M_T\right) \tag{18}$$

$$\varepsilon_{cV} = k_{cV} \exp\left(\frac{Q_{cV}}{RT}\right) F_{cV}\left(M_T\right) \tag{19}$$

$$\dot{x}_V^{+} = \frac{\dot{\varepsilon}}{\varepsilon_{cV}} \tag{20}$$

$$\dot{S}_{sbV}^{-} = \dot{S}_{bV}^{+} = \left(k_{NV} + k_{NB} S_B^p\right) \dot{\varepsilon} \left(x_V - 1\right) S_{sbV} \tag{21}$$

$$\dot{x}_V^{-} = x_v \frac{\dot{S}_{sbV}^{-}}{S_{sbV}} \tag{22}$$

The actual distribution of disorientation of sub-boundaries is thus not calculated, in contrast to the approach presented in Reference 10, in order to increase computation speed, reduce memory requirements, and enable model application for large 3D-FEM problems. However, the normalized non-dimensional values x and x_v can be understood as related to the fraction of sub-boundaries that approach

the critical 15° disorientation required for boundary migration to occur. Nucleation is assumed to start when the disorientation levels x or x_v become greater than 1, *i.e.*, when the critical deformation given by Equation (19) is reached (for x_v); there is an equivalent equation for x. In other words, when x or x_v reach the normalized value of 1, the most highly disoriented sub-boundaries are about to reach the 15° critical disorientation, and Equation (21), which expresses the potential of transition from sub-boundaries to mobile, high-angle grain boundaries, is about to be activated through the term (x_v-1). The fraction of sub-boundaries that reach the critical disorientation value and the potential for the transition from sub-boundaries to high angle boundaries (i.e., for nucleation) depends on how much the value x or x_v exceeds 1. Equation (22) is used to limit the increase of disorientation levels so that a dynamic equilibrium can be reached.

In Equation (21), S_B denotes the surface of intragranular recrystallized areas that develop around PSN sites (inside the initial grains). Such areas provide locations for subsequent additional nucleation (after the PSN particles themselves nucleate recrystallization as described by the parameter k_{NV}). This description suggests that volume and necklace nucleation could be described in a more unified manner once the first PSN recrystallized grains have formed.

F_V and F_{cV} are functions that depend on the Taylor factor of the particular MSU. Their value is taken to be unity for the Taylor factor of a wrought microstructure which exhibits a random texture (i.e., 3.06), whose kinetics are taken as reference. As a consequence, these functions express the increase or decrease of sub-boundary generation and disorientation rate as a function of the Taylor factor. Only sub-boundary generation and disorientation were deduced to depend on the crystallographic orientation in the model from the fitting process on experimental data. Actually, in most of the cases which were investigated, this dependence was weak (with a maximum ±10% variation), although such small variations are enough to noticeably affect the response of the material. One specific case exhibited the strongest effect of crystallographic orientation leading to increases of not just 10 but 100-150 pct., i.e., for the case of columnar grains in ingot microstructures whose axis (and <100> direction) was parallel to the compression axis, the critical deformation to start nucleation was a factor of 2 to 2.5 times higher for periphery and volume sub-boundaries, respectively, compared to the values for an isotropic material. In the present work, this was interpreted as due to the stability of the <100> fiber in uniaxial compression more than solely to considerations of stored energy. However, crystal-plasticity FEM might provide further, useful insight for this part of the modeling formalism.

Solution Method

The meso-scale, mechanism based model formulation was implemented using RX-MOD, a computer program for the modeling of dynamic and metadynamic recrystallization. The primary module of this software stores the experimental data used to fit the model parameters as well as subsequent model predictions. A second module generates the strain, strain-rate, temperature, time history corresponding to each set of experimental data. This includes an estimate of the temperature transients due to deformation heating, the precise delay time between the end of deformation and quenching (even for samples which were quenched with no nominal dwell time), and so forth. A microstructure-evolution module performs the numerical integration of the model on this thermomechanical path. An optimization module performs a fitting process used to reduce the average error in the model predictions by modifying the model parameters within specified, physically-realistic, limits. Last, a graphic post-processor allows the user to visualize those processing conditions for which the model needs be improved.

The current modeling approach was applied initially to laboratory-generated data for Waspaloy of various types (i.e., single hit with or without post-deformation dwell prior to quenching, ingot vs wrought preform microstructure). A comparison of measured and predicted (fitted) values of the recrystallized fraction gave an average error of 9.5 volume pct. (Figure 4). However, the magnitude of

the error varied with the type of preform microstructure and test. For a fine, equiaxed wrought microstructure which underwent recrystallization dynamically and metadynamically (with 0 to 30 s post-deformation hold times), the average error was ~7.3 volume pct. Similarly, for samples with the coarse, ingot microstructure quenched as quickly as possible after deformation (i.e., within ~2-3 s), a comparable discrepancy was observed. On the other hand, the average error for ingot material subjected to moderate to long post-deformation dwell periods of metadynamic recrystallization (lasting from 30 s to 1 h), the average error depended on the compression direction relative to the columnar-grain direction/fiber axis, i.e., the Taylor factor (Figure 4). When the columnar-grain direction was *parallel* to the compression axis, for which the Taylor factor is lowest, the difference between measured and predicted recrystallized fractions was only slightly greater than that for the previously-discussed situations. When the columnar grains were compressed in the *transverse* direction, the scatter increased. The worst agreement was found for the case in which the grain axis lay at 45° to the compression axis, for which the average Taylor factor was highest (3.66). Part of the discrepancy may come from inadequate sampling in the experiments due to the coarse grain structure in ingot samples, despite the fact that relatively large areas were characterized. Future work will focus on obtaining a better understanding of the effect of local texture and misorientation of neighboring grains on the evolution of substructure and recrystallization.

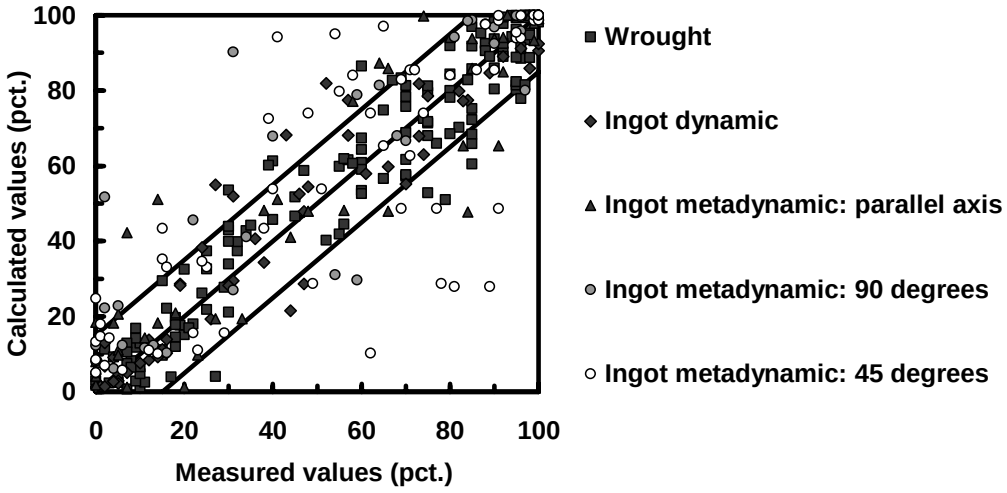

Figure 4. Comparison of measured and predicted recrystallized fractions.

III. Application to the Ingot-Cogging Process

The RX-MOD software was enhanced to enable the input of thermomechanical paths generated from 3D FEM simulations of hot working processes using the commercial code DEFORM-3D™. Attention was focused on ingot-cogging as an initial (and industrially-important) example. Such simulations are especially challenging from the standpoint of calculation and memory requirements because of the large number of nodes (in the thousands) and strain increments (in the hundreds) and thus the very large amount of data that is generated and must be saved. The memory requirements are exacerbated by the need to store microstructure information at each node as well. For the cogging problem, therefore, it was not possible to refine the entire FEM mesh too much, or the simulation time would have increased dramatically. Hence, the imported mesh was refined selectively (Figure 5a). This refinement did not increase the accuracy of temperature and deformation gradients, but enabled more accurate determination of the effect of the field variables on microstructure evolution for regions such as the ingot periphery at which the microstructure is only partially recrystallized (Figure 5b).

Several challenges remain to be addressed. First, the relatively complex microstructure in the different areas of a superalloy ingot must be input. These regions include the equiaxed (chill-zone) grains at the

periphery, the axial, columnar grains at the bottom, and the columnar grains oriented at 45° in other areas. Such a refinement is needed for the determination of the local Taylor factor (as a function of the local texture and strain-rate tensor) used as input to the microstructure model. The inclusion of additional MSUs to treat different generations of recrystallized and/or growing grains is another enhancement that is especially important for ingot cogging because of the complex deformation and reheating schedules used in this process.

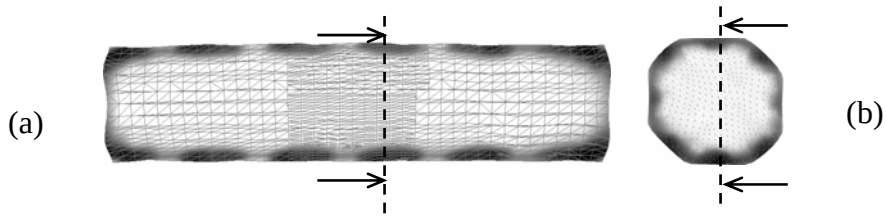

Figure 5. Model predictions of recrystallized fraction for the (a) longitudinal and (b) transverse sections of an ingot after eight passes and one reheat. (Lighter means higher recrystallized fraction.)

IV. Conclusions

A novel meso-scale, mechanism-based model of microstructural evolution was designed and tested. It combines advantages of both Avrami-based models, owing to its relatively simplicity and averaging over grain populations performed within a straightforward geometric framework, and cellular automata, inasmuch as it incorporates physically-representative parameters and driving forces. This modeling method appears to be promising with regard to providing a useful new tool for industrial process design. However, several fundamental and practical challenges require further work. These include improved physics-based descriptions of substructure evolution and modifications to the application software to allow more flexibility with regard to the definition of MSUs.

Acknowledgements- This work was conducted as part of the in-house research activities of the Metals Processing Group of the Air Force Research Laboratory's Materials and Manufacturing Directorate. The support and encouragement of the Laboratory management and the Air Force Office of Scientific Research (Dr. J.S. Tiley, program manager) are gratefully acknowledged. Technical discussions with Professor F. Montheillet (Ecole des Mines de Saint-Etienne) and the yeoman assistance of P.N. Fagin in conducting the experimental work are also much appreciated. One of the authors (JP Thomas) was supported through Air Force Contract F33615-03-D-5801.

References

1. S.L. Semiatin, D.S. Weaver, P.N. Fagin, M.G. Glavicic, R.L. Goetz, N.D. Frey, R.C. Kramb and M.M. Anthony, *Metal. Mater. Trans. A*, 2004, vol. 35A, pp 679-693
2. J.Ph. Thomas, F. Montheillet and S.L. Semiatin, submitted to *Metal. Mater. Trans. A*, 2006
3. G. Shen, S.L. Semiatin and R. Shivpuri, *Metal. Mater. Trans. A*, 1995, vol. 26A, pp 1795-1803
4. A. Laasraoui and JJ. Jonas, *Acta Mater.*, 1991, vol. 47, pp 4695-4710
5. B. Marty, J.Y. Guedou, P. Gergaud and J.L. Lebrun, *Superalloys 718, 625, 706 and Various Derivatives*, Ed. E.A. Loria, TMS, 1997, pp 331-342
6. C. Escher and G. Gottstein, *Acta Mater.*, 1998, vol. 46, pp 525-539
7. T. Sakai, *John J. Jonas Symposium on Thermomechanical Processing of Steel*, Ed. S. Yue and E. Essadiqi, CIM, 2000, pp 47-62
8. H.J. McQueen, *Mater. Sci. Eng. A*, 1988, vol. A101, pp 149-160
9. E.I. Poliak and J.J. Jonas, *Acta Mater.*, 1996, pp 127-136
10. J.Ph. Thomas, E. Bauchet, Ch. Dumont and F. Montheillet, *Superalloys 2004*, TMS, 2004, pp 959-968